Here is the theoretical part of Diffusion Model.

1 Langevin SDE

The Langevin SDE has the following form:

$$X_{t+s} = X_t + \nabla \log p_t(x_t)s + \sqrt{2s}\xi \tag{1}$$

where $X_t \in \mathcal{R}^d, p_t(x_t) = p(X_t = x_t)$, $\xi \sim N(0, I)$, I is identical matrix of $m \times m$. Our goal is to sample from specific $p(x,t)$.

Theorem 1 *The density of Langevin Diffusion Model converges to $p(x)$ over time. In other words, if $X_t \sim p(x)$, then $X_{t+s} \sim p(x)$ for $\forall s > 0$.*

Proof 1 *Let $\mu_t(f) = E\left[f\left(X_t\right)\right]$. Consider $\mu_{t+\tau}(f) = E\left[f\left(X_{t+\tau}\right)\right]$, as $\tau \to 0$. Then*

$$\begin{aligned}
\mu_{t+\tau} =& E\left[f\left(X_t + \nabla \log p_t\left(x_t\right) \cdot \tau + \sqrt{2\tau}\xi\right)\right] \\
=& E\left[f\left(x_t\right) + \nabla^\top f\left(x_t\right)\left(\tau \nabla \log p_t\left(x_t\right) + \sqrt{2\tau}\xi\right)\right. \\
&+ \left.\frac{1}{2}\left(\nabla^\top \log p_t(x_t)\tau + \sqrt{2\tau}\xi\right)\nabla^2 f(x_t)\nabla \log p_t(x_t)\tau + \sqrt{2\tau}\xi\right] \\
=& E\left[f\left(x_t\right)\right] + E\left[\tau \nabla^\top f\left(x_t\right)\nabla \log p_t\left(x_t\right)\right] \\
&+ \frac{\tau^2}{2}E\left[\nabla^\top \log p\left(x_t\right) \cdot \nabla^2 f\left(x_t\right) \cdot \nabla \log p\left(x_t\right)\right] + E\left[\tau \xi^\top \nabla^2 f\left(x_t\right)\xi\right]
\end{aligned} \tag{2}$$

The second term:

$$\begin{aligned}
&\tau E\left[\nabla^\top f \cdot \nabla \log p_t\right] \\
=& \tau \int \nabla f \cdot \nabla \log p_t p_t dx = \tau \int \nabla f \cdot \nabla p_t dx \\
=& -\tau \int \operatorname{tr}\left(\nabla^2 f\right) \cdot p_t dx = -\tau E\left[\operatorname{tr}\left(\nabla^2 f\right)\right] \\
=& -\tau E\left[\xi^\top \nabla^2 f \xi\right]
\end{aligned} \tag{3}$$

Then

$$\mu_{t+\tau} = E\left[\frac{1}{2}\nabla^\top \log p_t \nabla^2 f \nabla \log p_t\right] \cdot \tau^2 = O\left(\tau^2\right) \tag{4}$$

Hence we have $\frac{d}{dt}(\mu_t) = 0$, i.e. $E[\mu_t] = E[\mu_{t+s}]$ for $\forall s > 0$.

Remark 1 *We define the density of normal distribution $N(x;\mu,\Sigma)$, and its log-density, gradient of density and score as follows:*

$$\begin{cases}
N(x;\mu,\Sigma) = \dfrac{1}{\sqrt{(2\pi)^d|\Sigma|}}e^{-\frac{1}{2}(x-\mu)^\top\Sigma^{-1}(x-\mu)} \\
\log N(x;\mu,\Sigma) = -\dfrac{1}{2}(x-\mu)^\top\Sigma^{-1}(x-\mu) - \log\left(\sqrt{(2\pi)^d|\Sigma|}\right). \\
\nabla_x N(x;\mu,\Sigma) = N(x;\mu,\Sigma)\Sigma^{-1}(x-\mu) \\
\nabla_x \log N(x;\mu,\Sigma) = -\Sigma^{-1}(x-\mu).
\end{cases} \tag{5}$$

Actually, Langevin SDE is not necessary be as above i.e. the diffusion term is not necessary to be $\sqrt{2}$. The reason is to guarantee the stationary distribution of $p_t(x)$. i.e. the term $\frac{\partial p(x,t)}{\partial t} = 0$ in FPK equation. If the diffusion term is $g(t)$, then by FPK equation, we have

$$\nabla_x \cdot (fp - \frac{1}{2}g^2(t)\nabla p) = 0$$

then $f(x,t) = \frac{1}{2}g^2(t)\frac{\nabla_x p(x,t)}{p(x,t)} = \frac{1}{2}g^2(t)\nabla_x \log p(x,t)$.

2 Linear SDE

Then we consider linear SDE having the form:

$$dX_t = (a(t)X_t + b(t))dt + g(t)dW_t \tag{6}$$

By Euler Maruyama method, it can be approximated By

$$\begin{aligned} X_{t+s} &= X_t + (a(t)X_t + b(t))s + g(t)\sqrt{s}\xi \\ &= (1 + a(t)s)X_t + b(t)s + g(t)\sqrt{s}\xi \end{aligned} \tag{7}$$

where $\xi \sim N(0,1)$. Usually we need to consider the expectation, variance and distribution of x. But the stochastic value of x is dependent of x_0. Then first we consider

$$\begin{aligned} E\left[X_{t+s}|X_0\right] - E\left[X_t|X_0\right] &\approx \big(a(t)E\left[X_t|X_t\right] + b(t)s + g(t)\sqrt{s}E[\xi] \\ &= \left(a(t)E\left[X_t|X_0\right] + b(t)\right)s. \end{aligned} \tag{8}$$

Note $e(t) = E\left[X_t|X_0\right]$, then

$$e'(t) = \lim_{s\to 0} \frac{E\left[X_{t+s}|X_0\right] - E\left[X_t|X_0\right]}{s} = a(t)\cdot e(t) + b(t). \quad e(0) = X_0. \tag{9}$$

which is an ODE system, having solution

$$e(t) = \left(X_0 + \int_0^t e^{-\int_0^s a(r)dr} b(s)ds\right)\cdot e^{\int_0^t a(s)ds} \tag{10}$$

Therefore

$$\begin{aligned} E\left[X_t\right] &= E\left[E\left[X_t|X_0\right]\right] = E[e(t)] \\ &= \left(E\left[X_0\right] + \int_0^t e^{-\int_0^s a(r)dr} b(s)ds\right) e^{\int_0^t a(s)ds} \end{aligned} \tag{11}$$

Similarly, Note $\operatorname{Var}\left(X_0|X_0\right) = v(t)$: then $\operatorname{Var}\left(X_{t+s}|X_0\right) = (1+sa(t))^2 \operatorname{Var}\left(X_t|X_0\right) + sg^2(t)$. Then

$$\begin{aligned} V'(t) &= \lim_{s\to 0} \frac{\operatorname{Var}\left(X_{t+s}|X_0\right) - \operatorname{Var}\left(X_t|X_0\right)}{s} \\ &= \left[\left(a^2(t)s + 2a(t)\right)v(t) + g^2(t)\right]|_{s\to 0} \\ &= 2\alpha(t)V(t) + g^2(t), \qquad V(0) = 0 \end{aligned} \tag{12}$$

Solution is:

$$v(t) = \left(\int_0^t e^{-\int_0^s 2a(r)dr} g^2(s)ds\right) \tag{13}$$

By law of total variance

$$\begin{aligned} \operatorname{Var}\left(X_t\right) =& E\left[X_t^2\right] - E^2\left[X_t\right] = E\left[E\left[X_t^2|X_0\right]\right] - E^2\left[X_t\right] \\ =& E\left[\operatorname{Var}\left(X_t|X_0\right) + E^2\left[X_t|X_0\right]\right] - E^2\left[X_t\right] \\ =& E\left[\operatorname{Var}\left(X_t|X_0\right)\right] + E\left[E^2\left[X_t|X_0\right]\right] - E^2\left[E\left[X_t|X_0\right]\right] \\ =& E\left[\operatorname{Var}\left(X_t|X_0\right)\right] + \operatorname{Var}\left(E\left[X_t|X_0\right]\right) \end{aligned} \tag{14}$$

then

$$\begin{aligned} \operatorname{Var} =& E[V(t)] + \operatorname{Var}(e(t)) \\ =& \left(\int_0^t e^{-\int_0^s 2a(r)dr} g^2(s)ds\right) e^{\int_0^t 2a(s)ds} + e^{\int_0^t 2a(s)ds}\cdot \operatorname{Var}\left(X_0\right). \end{aligned} \tag{15}$$

We have the following theorem which is crucial for diffusion models.

Theorem 2 *If* $X_{t+s} = (1 + a(t)s)X_t + b(t)s + g(t)\sqrt{s}\xi$
then $X_t|X_0 \sim N\left(E\left[X_t|X_0\right], \operatorname{Var}\left(X_t|X_0\right)\right)$*, where* $\left(E\left[X_t|X_0\right] = e(t), \operatorname{Var}\left(X_t|X_0\right) = V(t)\right)$.

Next, we will see how the above formula can be applied to diffusion modtels. There are three frameworks to build SDEs for diffusion models, VP, VE and sub-VP.

Definition 1 *Noise function* $\beta(t)$ *. s.t.* $\beta(0) = 0; \beta'(t) \geqslant 0; \beta(t) \to \infty$ *as* $t \to \infty$

2.1 Variance Preserving (VP) SDE

So if we have diffusion model like:

$$\begin{aligned} X_{t_{i+1}} &= \sqrt{1 - \left(\beta\left(t_{i+1}\right) - \beta\left(t_i\right)\right)} X_{t_i} + \sqrt{\left(\beta\left(t_{i+1}\right) - \beta\left(t_i\right)\right)}\xi \\ &= \sqrt{1 - \Delta\beta(t_i)} X_{t_i} + \sqrt{\Delta\beta(t_i)}\xi \end{aligned} \tag{16}$$

Then the conditional distribution is given by:

$$q\left(X_{t_{i+1}}|X_{t_i}\right) = N(x_{t_{i+1}}; \sqrt{1 - \Delta\beta\left(t_i\right)} X_{t_i}, \Delta\beta\left(t_i\right)) \tag{17}$$

Then we need to estimate θ drift term f and diffusion term g:

$$\begin{aligned} f(x,t) &= \lim_{h \to 0} \frac{E\left[X_{t+h} - X_t | X_t = x\right]}{h} \\ &= \lim_{h \to 0} \frac{x\sqrt{1 - \Delta\beta(t)} - x}{h} = -\frac{x}{2}\beta'(t). \\ g(t) &= \sqrt{\lim_{h \to 0} \frac{N\left[X_{t+h}|X_t = x\right]}{h}} = \sqrt{\lim_{h \to 0} \frac{\beta(t+h) - \beta(t)}{h}} = \sqrt{\beta'(t)} \end{aligned} \tag{18}$$

Then the model can be written as $dx = -\frac{x}{2}\beta'(t)dt + \sqrt{\beta'(t)}dW_t$

Then by Theorem 2 we have

$$\begin{cases} E\left[X_t|X_0\right] = X_0 e^{\int_0^t -\frac{1}{2}\beta'(s)ds} = X_0 e^{-\frac{1}{2}\beta(t)} \\ E\left[X_t\right] = E\left[X_0\right] e^{-\frac{1}{2}\beta(t)} \\ V\left(X_t|X_0\right) = \displaystyle\int_0^t e^{\int_0^s \beta'(r)dr}\beta'(s)ds \cdot e^{-\beta(t)} = 1 - e^{-\beta(t)} \\ V\left(X_t\right) = 1 - e^{-\beta(t)} + V\left(X_0\right)e^{-\beta(t)} = 1 + \left(V\left(X_0\right) - 1\right)e^{-\beta(t)}. \end{cases} \tag{19}$$

So as $t \to \infty, \beta(t) \to \infty$, then $E \to 0, V \to 1$, i.e. $X_t|X_0 \sim N\left(E\left[X_t|X_0\right], \operatorname{Var}\left|X_t\right| X_0\right) \to N(0,1)$ as $t \to \infty$.

2.2 Variance-Exploding SDE

Here is the model: $X_{t+h} = X_t + \sqrt{\Delta\beta(t)}\xi$

Similarly we can compute the $f(x,t) \equiv 0$ and $g(t) = \sqrt{\beta(t)}$. Hence

$$\begin{cases} E\left[X_0|X_0\right] = X_0 \\ E\left[X_t\right] = E\left[X_0\right] \\ V\left(X_t|X_0\right) = \displaystyle\int_0^t e^{\int_0^s 0dr}\beta'(s)ds = \beta(t) \\ V\left(X_t\right) = V\left[X_0\right] + \beta(t) \end{cases} \tag{20}$$

So the expectation value is constant and the variance is increasing monotonical.

If we rescale X_t as $Y_t = \frac{X_t}{\sqrt{\beta(t)}}$, then $Y_t \to N(0,1), t \to \infty$.

2.3 Sub-VP SPE

Here, we set the dift and diffusion term as

$$\begin{aligned} f(x,t) &= -\frac{1}{2}\beta'(t) \\ g(t) &= \sqrt{\beta'(t)\left(1-e^{-2\beta(t)}\right)} \end{aligned} \tag{21}$$

As the same, we can compute that.

$$\begin{cases} E\left[X_t|X_0\right] = X_0 e^{-\frac{1}{2}\beta(t)} \\ E\left[X_t\right] = E\left[X_0\right] e^{-\frac{1}{2}\beta(t)} \\ V\left(X_t|X_0\right) = \left(1-e^{-\beta(t)}\right)^2 \\ V\left(X_t\right) = \left(1-e^{-\beta(t)}\right)^2 + V\left(X_t\right) e^{-\beta(t)}. \end{cases} \tag{22}$$

We can find out that the variance is always smaller thar VP SDE.

Remark 2 *To sum up, finally we hope that X_t converges to a normal distribution by choosing different drift and diffusion functions. For generative model, the goal is to sample from a Data distribution p_{data}. We have known that if we set the initial distribution $p_0(x_0) = p(X_0 = x_0) \sim p_{data}$, then after $t = T$, the distribution of X_t is tend to be $N(0,1)$ under certain conditions.*

So the idea is backward: if we sample from $X_T \sim N(0,1)$, and then run SDE backwards, could we get the initial distribution?

3 Reverse SDE

Assume we have forward SDE: from $X_0 \sim p_0, X_T \sim p_T$,

$$dX_t = f(X_t,t)dt + g(t)dW_t \tag{23}$$

Then we define the reverse SDE as: from $X_T \sim p_T$,

$$d\bar{X}_t = \bar{f}(\bar{X}_t,t)dt + \bar{g}(t)d\bar{W}_t \tag{24}$$

where $\bar{W}_t$ is Brownian Motion runns backward in time, i.e. $\bar{W}_{t-s} - \bar{W}_t$ is independent of $\bar{W}_t$. We can approximate by EM:

$$\bar{X}_{t-s} - \bar{X}_t = -s\bar{f}(\bar{X}_t,t) + \sqrt{s}\bar{g}(t)\xi \tag{25}$$

So the problem is: If given f, g, are there $\bar{f}, \bar{g}$ s.t. the reverse time diffusion process $\bar{X}_t$ has the same distribution as the forward process X_t? Yes!

Theorem 3 *The reverse SDE with $\bar{f}, \bar{g}$ having the following form has the same distribution as the forward SDE 23:*

$$\begin{cases} \bar{f}(x,t) = f(x,t) - g^2(x,t)\dfrac{\partial}{\partial x}\log p_t(x) \\ \bar{g} = g(t) \end{cases} \tag{26}$$

i.e.

$$d\bar{X}_t = \left[f(\bar{X}_t,t) - g^2(t)\log p_t(x_t)\right]dt + g(t)d\bar{W}_t \tag{27}$$

Proof 2 *The proof is skipped.*

This theroem allows us to learn how to generate samples from p_{data}.

Algorithm 1 *:*
Step1. Select $f(x,t)$ and $g(t)$ with affine drift coefficients s.t. $X_T \sim N(0,1)$
Step2. Train a network $s_\theta(x,t) = \frac{\partial}{\partial x}\log p_t(x)$ where $p_t(x) = p(X_t = x)$ is the forward distribution.
Step3. Sample X_T from $N(0,1)$, then run reverse SDE from T to 0:

$$\bar{X}_{t-s} = \bar{X}_t + s\left[g^2(t)s_\theta(\bar{X}_t,t) - f(\bar{X}_t,t)\right] + \sqrt{s}g(t)\xi \tag{28}$$

4 Loss function

Normally we can define the loss function as follows:

$$\begin{aligned} L_\theta &= \frac{1}{T}\int_0^T \lambda(t) \underset{x_0\sim p_{data}}{E}\left[\underset{x_t\sim p_{t|0}(x_t|x_0)}{E}\left[\|s_\theta(x_t,t) - \nabla_{x_t}\log p_t(x_t)\|^2\right]\right]dt \\ &= \underset{t\sim U(0,T)}{E}\left[\lambda(t)\underset{x_0\sim p_{data}}{E}\left[\underset{x_t\sim p_{t|0}(x_t|x_0)}{E}\left[\|s_\theta(x_t,t) - \nabla_{x_t}\log p_t(x_t)\|^2\right]\right]\right] \end{aligned} \tag{29}$$

It should be clearified that $p_{t|0}(x_t|x_0) = p(X_t = x_t|X_0 = x_0)$. So

$$p_t(x_t) = \int p_{t|0}(x_t|x_0)p_0(x_0)dx_0 = E_{x0\sim p_{data}}\left[p_{t|0}(x_t|x_0)\right]$$

. Then $p_t(x) = p\left(X_t = x\right)$. $\quad p_{t|0}(x|y) = p\left(X_t = x|x_0 = y\right)$.

$$\begin{aligned} \nabla\log p_t(x) &= \frac{1}{p_t(x)}\nabla p_t(x). \\ &= \frac{1}{p_t(x)}\nabla\int p_{t|0}(x|y)p_0(y)dy \\ &= \frac{1}{p_t(x)}\int \nabla p_{t|0}(x|y)p_0(y)dy \\ &= \frac{1}{p_t(x)}\int \frac{\nabla p_{t|0}(x|y)}{p_{t|0}(x|y)}p_0(y)\cdot p_{t|0}(x|y)dy \\ &= \int \nabla_x\log\left(p_{t|0}(x|y)\right)\cdot p_{0|t}(y|x)dy \\ &= E_y\left[\nabla_x\log\left(p_{t|0}(x|y)\right)\right] \end{aligned} \tag{30}$$

Lemma 1 *If $y \sim p_{0|t}(y|x), x \sim p_t(x)$, then $y \sim p_0(y)$*

Proof 3

$$\begin{aligned} p\left(x_0 = y|x_t = x\right) = \int p\left(x_0 = y|x_t = x\right)p\left(x_t = x\right)dx = \int p\left(x_t = x|x_0 = y\right)p\left(x_0 = y\right)dx. \\ = p\left(x_0 = y\right) = p_{data}\left(y\right) \end{aligned} \tag{31}$$

Then we can rewrite the loss function as:

$$\begin{aligned} L_\theta &= \underset{t\sim U(0,T)}{E}\left[\lambda(t)\underset{x_0\sim p_{data}}{E}\left[\underset{x_t\sim p_{t|0}(x_t|x_0)}{E}\left[\left\|S_\theta\left(x_t,t\right) - \frac{\partial}{\partial x_t}\log p_t\left(x_t\right)\right\|^2\right]\right]\right] \\ &\leqslant \underset{t\sim U(0,T)}{E}\left[\lambda(t)\underset{x_0\sim p_{data}}{E}\left[\underset{x_t\sim p_{t|0}(x_t|x_0)}{E}\left[\underset{y\sim p_{data}}{E}\left[\left\|S_\theta\left(x_t,t\right) - \nabla_{x_t}\log p_{t|0}(x|y)\right\|^2\right]\right]\right]\right] \\ &= \underset{t\sim U(0,T)}{E}\left[\lambda(t)\underset{x_0\sim p_{data}}{E}\left[\underset{x_t\sim p_{t|0}(x_t|x_0)}{E}\left[\|S_\theta\left(x_t,t\right) - \nabla_{x_t}\log\left(p_{t|0}\left(x_t|x_0\right)\|^2\right]\right]\right]\right. \end{aligned} \tag{32}$$

Since $p_{t|0}\left(X_t|x_0\right) = p\left(X_t = x_t|X_0 = x_0\right)$ has been discussed:

$$p_{t|0}\left(x_t|x_0\right) \sim N\left(x_t; E\left[X_t = x_t|X_0 = x_0\right], \operatorname{Var}\left(X_t = x_t|X_0 = x_0\right)\right).$$

Then by theorem 2

$$\frac{\partial}{\partial x}\log p_{t|0}\left(x|x_0\right) = -\frac{x - E_{t|0}\left[x|x_0\right]}{\mathrm{Var}_{t|0}\left(x|x_0\right)} = -\frac{x - e(t)}{V(t)} \tag{33}$$

So

$$\begin{aligned} L_\theta &= \underset{t\sim U(0,T)}{E}\left[\lambda(t)\underset{x_0\sim p_{data}}{E}\left[\underset{\xi\sim N(0,1)}{E}\left[\left\|s_\theta\left(\sqrt{\mathrm{Var}_{t|0}(x_t|x_0)}\xi + E_{t|0}[x_t|x_0], t\right) + \frac{\xi}{\sqrt{\mathrm{Var}_{t|0}(x_t|x_0)}}\right\|^2\right]\right]\right] \\ &= \underset{t\sim U(0,T)}{E}\left[\lambda(t)\underset{x_0\sim p_{data}}{E}\left[\frac{1}{\mathrm{Var}_{t|0}(x_t|x_0)}\underset{\xi\sim N(0,1)}{E}\left[\left\|\xi_\theta\left(\sqrt{\mathrm{Var}_{t|0}(x_t|x_0)}\xi + E_{t|0}[x_t|x_0], t\right) - \xi\right\|^2\right]\right]\right] \end{aligned} \tag{34}$$

where $\xi_\theta = -s_\theta\sqrt{\mathrm{Var}_{t|0}(x_t|x_0)}$ is called denoising network.